

Gold Gap Energy

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Abstract: The gap energy of gold has been calculated and compared to the adsorption energy.

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1. INTRODUCTION

With the help of distribution and alignment energy let us calculate the gap energy of gold 5d electrons [1].

2. THE ORIGINAL GOLD ORBIT ENERGY

The original gold 5d orbit length $s_{original}^{5d Au}$ and the corresponding kinetic energy of the electron $Wk_{original}^{5d Au}$ are related to the effective nuclear charge $Z_{effective}^{5d Au}$ belonging to 5d electrons [2] which covers the nuclear charge as well as the shielding effect committed by the neighbouring electrons.

The original gold 5d orbit length is expressed in Compton wavelengths of the electron as follows [1], [2]:

$$s_{original}^{5d Au} = \frac{\alpha^{-1}}{Z_{effective}^{5d Au}} = \frac{137.035\ 999\ 084}{20,126} = 6,808\ 903\ 860. \quad (1)$$

And the original gold 5d orbit kinetic energy of the electron is the next [1], [2]:

$$Wk_{original}^{5d Au} = Z_{effective}^{5d Au} \cdot Ry = 20,126 \times 13.605\ 693\ 122\ 994\ eV = 273,828\ 179\ 793\ 377\ eV. \quad (2)$$

3. THE GOLD DISTRIBUTION ENERGY

The original gold 5d orbit length (1) does not satisfy the restrictions of the double surface geometry [1], but so do the distributed orbits around it:

$$s_{5d Au}(n) = n \left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}} \right), \quad 1 \leq n \in \mathbb{N} \leq 14 \quad (3)$$

The electron on different distributed orbits has the same total energy but different kinetic energy [1]:

$$Wk_{5d Au}(n) = Wk_{original}^{5d Au} \left(2 \frac{s(6)}{s(n)} - 1 \right) = Wk_{original}^{5d Au} \left(2 \frac{6(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{(6)^2}}})}{n(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}})} - 1 \right), \quad 1 \leq n \in \mathbb{N} \leq 14. \quad (4)$$

There are thus fourteen quantized distributed gold 5d orbit lengths and 14 kinetic energies of the electron (distribution energies). Because of an unstable original orbit $s_{original}^{5d Au} = 6,808\ 903\ 860 \approx s(6) = 6,684\ 550\ 414 \dots$ the electron on the sixth distributed orbit is considered to take over the unchanged original kinetic energy (2):

$$Wk_{5d Au}(6) = Wk_{original}^{5d Au} = 273,828 \text{ eV}. \quad (5)$$

The electron on the penultimate, i.e. 13th orbit possesses the next distribution energy:

$$Wk_{5d Au}(13) = 21,609 \text{ eV}. \quad (6)$$

And the electron on the last, i.e. 14th orbit possesses the next distribution energy:

$$Wk_{5d Au}(14) = 0,110 \text{ eV}. \quad (7)$$

4. THE GOLD ALIGNMENT ENERGY

The alignment energy is the kinetic energy of the electron enabling the alignment of the atom wave nature inside the electron wave nature. It is given by the next formula:

$$Wk_{alignment} = \left(\frac{R_{unaligned}}{R_{aligned}} - 1 \right) m_{electron}^{rest} c^2. \quad (8)$$

For gold we have[3], [4]:

$$R_{unaligned}^{Au} = \frac{m_{Au}}{m_{electron}^{rest}} s(1) = \frac{196,966\ 570 \text{ Da}}{0,00054857990907 \text{ Da}} 1,696\ 685\ 529 = 609\ 191,7030. \quad (9)$$

Thus the aligned whole-part ratio is

$$R_{aligned}^{Au} = s(609\ 191) = 609\ 191,000\ 008 \dots \quad (10)$$

And the gold alignment energy yields (8):

$$Wk_{alignment}^{Au} = 0,590 \text{ eV}. \quad (11)$$

5. THE GOLD GAP ENERGY

The gap energy is the smallest difference between the kinetic energy of the electron enabling the alignment of the electron by the atom and the nearest kinetic energy of the electron enabling the particular distribution of the electron in the atom. For gold - where the alignment energy lies between the distribution energies of the 13th and 14th orbit - we have (6), (7), (11):

$$W_{gap}^{Au} = Wk_{alignment}^{Au} - Wk_{5d Au}(13) = 0,590 \text{ eV} - 21,609 \text{ eV} = -21.02 \text{ eV}. \quad (12a)$$

And

$$W_{gap}^{Au} = Wk_{alignment}^{Au} - Wk_{5d Au}(14) = 0,590 \text{ eV} - 0,110 \text{ eV} = 0.48 \text{ eV}. \quad (12b)$$

6. CONCLUSION

The given positive gap energy $W_{gap}^{Au} = 0.48 \text{ eV}$ could have a role in adsorption process on Au surface where the valence states of small molecules (e.g. NO and CO) interact with the gold 5d orbits. Indeed, the above value equals the calculated adsorption energy of CO on the top site of Au surface as well as it is near the available reference value in literature which is in the range of 0.53–0.69 eV [5].

DEDICATION

This fragment is dedicated to Saint Anne (Sveta Ana) to shield the Municipality of Sveta Ana v Slovenskih goricah



Figure1. Saint Anne in Slovenske gorice

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